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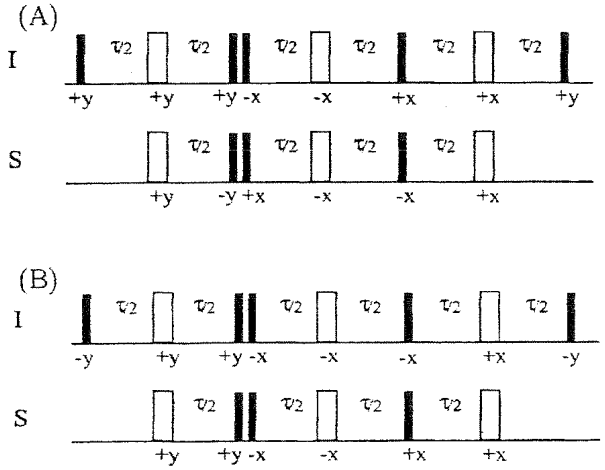
(54) Title: QUANTUM CELLULAR AUTOMATA COMPUTING WITH ENDOHEDRAL FULLERENES



(57) Abstract: Universal quantum computation is performed using global addressing techniques as applied to a physical system of spin entities of two distinct types arranged in an ABABAB sequence. Algorithms are provided for performing global unitary operations on such arrays and thereby providing a framework for performing any logical computations. Simple spin $\frac{1}{2}$ units such as free electrons are provided for, as well as molecular entities. The preferred system consists of an ABAB linear array of Group V endohedrally doped fullerenes which can be reliably manipulated and arrayed on silicon. Each molecule spin site consists of a nuclear spin coupled via a hyperfine interaction to an electron spin. The electron spin of each molecule is in a quartet ground state $S = 3/2$. Neighboring molecular electron spins are coupled via a magnetic dipole interaction. A quantum cellular automata quantum computing architecture is provided using these molecules by encoding the quantum information on the nuclear spins while using the electron spins as a local bus. The NMR and ESR pulses required to execute the basic cellular automata operations are described.

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QUANTUM CELLULAR AUTOMATA COMPUTING WITH ENDOHEDRAL FULLERENES

Technical Field

This invention relates to quantum computing methods, systems and apparatuses.

Background Art

Quantum information processing (QIP), relies on the ability to perform a selection of unitary operations on a multi-partite system. More precise criteria that must be met by any physical implementation of a quantum information processor have been proposed in [1] (see reference details at the end of the description). In particular, in a spin-based quantum computer architecture the spin sites (i) should be easy to physically manipulate, (ii) easy to replicate in numbers, (iii) they should possess some type of inter-site interaction and (iv) they also should be somewhat isolated from their environment.

Meeting such ideals in practice is very demanding. It is believed by some that a solid-state implementation could prove highly advantageous in terms of the scaling up of the number of spin sites and many solid-state proposals for a quantum information processor are currently under study [3,5,4]. However, to achieve (iv), usually requires the spin-sites to be located within a near-perfect crystal lattice and this leads to great difficulties in satisfying (i) and (ii) above.

If the interaction between spin sites is mediated by a predominantly electronic interaction, as is the case in ion-trap quantum computers and [3], the quantum computer operation will be very sensitive to stray electric charges. Such systematic charge noise can be source of heating and may be very difficult to eliminate.

Additionally the use of local qubit addressing is ubiquitous in very many quantum computer designs. However the use of such local qubit addressing comes with a potentially very large overhead such as the building of nanoscopic metal gates as in [3], or the greatly increased bandwidth required in NMR quantum computing in order to frequency address a large number of spins in a molecule [2]. For small numbers of qubits, this overhead may be acceptable but

the decoherence effects of imperfect local addressing in a device containing many tens of qubits may be much more serious.

Finally, the use of nuclear spins alone in a spin-based quantum computer design leads to a serious difficulty in achieving a sufficiently high initial spin polarization with which to initialise the quantum computer. This is a primary obstacle in liquid state NMR quantum computing and the problem remains in solid-state designs even when the nuclei are cooled to milli-Kelvin temperatures.

Faced with all these challenges, the concept of encoding a qubit into the spin system contained within an endohedrally doped fullerene has been investigated [6,7]. In [7], the unusual properties of Group V C60 endohedral fullerenes are outlined and their potential use in a solid-state implementation is indicated. However, none of the prior art provides a quantum computing architecture for use with this material.

Disclosure of the Invention

The invention provides a method of quantum computing in a system comprising a plurality of spin systems of two distinct types A and B arrayed in an ABABAB... sequence, wherein each A-type spin system comprises a first spin subsystem A1 and a second spin subsystem A2 coupled to one another, and each B-type spin system comprises a first spin subsystem B1 and a second spin subsystem B2 coupled to one another, wherein the first spin subsystems (A1,B1) of neighbouring A and B-type spin systems are substantially isolated from one another and the second spin subsystems (A2,B2) of neighbouring A and B-type spin systems are coupled to one another, said method comprising the steps of:

a) encoding quantum information on the first spin subsystems (A1,B1); and
b) employing the second spin subsystems (A2,B2) as a local bus for the information encoded on the first spin subsystems.

The invention further provides a quantum computer comprising:

a) a plurality of entities providing quantum spin systems of two distinct types A and B arrayed in an ABABAB... sequence, wherein

each A-type spin system comprises a first spin subsystem A1 and a second spin

subsystem A2 coupled to one another, and each B-type spin system comprises a first spin subsystem B1 and a second spin subsystem B2 coupled to one another,

the first spin subsystems (A1,B1) of neighbouring A and B-type spin systems are substantially isolated from one another and the second spin subsystems (A2,B2) of neighbouring A and B-type spin systems are coupled to one another,

b) an NMR/ESR pulse generator associated with said array of entities for generating and applying said pulses to said array of entities; and

c) means for reading the spin state of one or more of said entities.

In another aspect the invention provides a method of quantum computing in a system comprising a plurality of spin systems of two distinct types $\mathcal{A}$ and $\mathcal{B}$ arrayed in an $\mathcal{AB}\mathcal{AB}\mathcal{AB}$ sequence, wherein each spin system comprises a spin ½ entity, said method comprising performing one or more global unitary operations $\hat{\mathcal{A}}_f^U$ on the $\mathcal{A}$ spin systems, wherein:

$\hat{\mathcal{A}}_f^U$ is the conditional application of the unitary U when $U \sim NOT$ to the $\mathcal{A}$ spins depending on the state of $\mathcal{A}$'s neighboring $\mathcal{B}$ spins;

f is the sum of the states of the neighboring $\mathcal{B}$ spins, with spin up(down) defined as 1(0) such that $f \in [0,1,2]$;

and wherein:

said global unitary operations are performed by applying pulse sequences according to one of the following sequence notations (a)-(c):

a) $\hat{\mathcal{A}}_2^U = \Xi(\mathcal{B}, A; \{X_\delta^{\mathcal{A}}\}) \cdot \{X_{\pi/2-\delta}^{\mathcal{A}}\} \cdot \{Z_{-\pi/2}^{\mathcal{A}}\} \cdot \Xi(\mathcal{B}, \mathcal{A}; \{X_\pi^{\mathcal{A}}\})\{Z_{-\pi/2}^{\mathcal{A}}\} \cdot \{X_{\pi/2-\delta}^{\mathcal{A}}\} \cdot \Xi(B, A; \{X_\delta^{\mathcal{A}}\})$. read from right to left where $2\delta = \theta$; or

b) $\hat{\mathcal{A}}_1^U =$ $\{Z_\pi^{\mathcal{A}}\}$ $\cdot \{X_{\pi/2-\delta}^{\mathcal{A}}\} \cdot \{Z_{-\pi/2}^{\mathcal{A}}\} \cdot \Xi(\mathcal{B}, \mathcal{A}; \{X_\pi^{\mathcal{A}}\})\{Z_{-\pi/2}^{\mathcal{A}}\} \cdot \{X_{\pi/2-\delta}^{\mathcal{A}}\} \cdot \Xi(B, A; \{X_\delta^{\mathcal{A}}\})$. read from right to left where $\delta = \theta$; or

c) $\hat{\mathcal{A}}_0^U$ implemented as an application of $\{X_\pi^{\mathcal{B}}\}$ to all the $\mathcal{B}$ spins, followed by $\hat{\mathcal{A}}_2^U$, followed by an application of $\{X_\pi^{\mathcal{B}}\}$ to all the $\mathcal{B}$ spins;

wherein the controlled operation of applying U to an $\mathcal{A}$ spin with left and right $\mathcal{B}$ neighbours such that the $\mathcal{B}$ spins control the unitary application is denoted by $C(\mathcal{B},\mathcal{A};U)$. and the function Ξ is in turn defined by the equation:

$$\Xi(\mathcal{B},\mathcal{A};U) \equiv C(\mathcal{B}_{\text{on the left}},\mathcal{A};U)C(\mathcal{B}_{\text{on the right}},\mathcal{A};U) \ ,$$

and wherein in equations (a)-(c) the NMR/ESR notation for $\pi/2$ pulses used is:

$$[+S_y^{\mathcal{B}}] \equiv \exp(i\frac{\pi}{2}S_y^{\mathcal{B}}) \ ,$$

and rotation through the angle γ about the $z-$axis, for example, is denoted as:

$$\{Z_\gamma^{\mathcal{A}}\} \equiv \exp(i\gamma S_z^{\mathcal{A}}) \ .$$

In this aspect of the invention there is also provided a quantum computer comprising:

a) a plurality of entities providing quantum spin systems of two distinct types A and B arrayed in an ABABAB... sequence, wherein each spin system comprises a spin ½ entity copled to its two neighbours

b) an NMR/ESR pulse generator associated with said array of entities for generating and applying said pulses to said array of entities; and

c) means for reading the spin state of one or more of said entities.

Brief Description of the Drawings

The invention will be further illustrated by the following descriptions of embodiments thereof given by way of example only with reference to the accompanying Drawings in which:

Figure 1A depicts the simulated NMR spectra of $\mathcal{A}$ =^{15}N@C60 and $\mathcal{B}$ =^{31}P@C60 with (a) and (b) labeling the spectral lines from $\mathcal{A}$ and $\mathcal{B}$ respectively;

Figure 1B depicts the simulated ESR spectra of $\mathcal{A}$ =^{15}N@C60 and $\mathcal{B}$ =^{31}P@C60 with (a) and (b) labeling the spectral lines from $\mathcal{A}$ and $\mathcal{B}$ respectively;

Figure 2 is a schematic depiction of the $\mathcal{AB}\mathcal{AB}\mathcal{AB}$ quantum cellular automata chain using the Group-V endohedral fullerenes;

Figures 3A to 3E collectively form a schematic representation of the steps (a)-(e) described below to execute the global operation $\hat{A}_I^U$ in a chain similar to that of Fig. 2, having the effect of flipping the state of the leftmost $\mathcal{A}$ nuclear qubit.

Figure 3A shows the S qubits in their ground state with some pattern of I qubits;

Figure 3B shows the result of a hyperfine *SWAP* of the quantum information in the $\mathcal{B}$ molecules;

Figure 3C shows the result of the conditional flipping of the $\mathcal{A}$ electronic qubit depending on the neighboring $\mathcal{B}$ electronic qubits;

Figure 3D shows the result of a hyperfine *SWAP* of the $\mathcal{B}$ qubits back into the nuclei;

Figure 3E shows a controlled global unitary operation U applied to the nuclei of all molecules conditioned by the state of their electronic qubits.

Figure 4A shows an NMR/ESR pulse sequence, in which the solid black bars are $\pi/2$ pulses while the white bars are refocusing π pulses, for a logical SWAP between spin $I = 1/2$ and the inner electronic qubits of spin $S = 3/2$ as described in equation 12 below;

Figure 4B shows an NMR/ESR pulse sequence, in which the solid black bars are $\pi/2$ pulses while the white bars are refocusing π pulses, for a logical SWAP between spin $I = 1/2$ and the outer electronic qubits of spin $S = 3/2$ as described in equation 13 below; and

Figure 5 shows an NMR/ESR pulse sequence, in which the black pulses are π pulses and the, to selectively couple $I^{\mathcal{B}}$ with $S^{\mathcal{B}}$ while decoupling $S^{\mathcal{A}}$ with $S^{\mathcal{B}}$, and simultaneously decoupling $S^{\mathcal{A}}$ with $I^{\mathcal{A}}$.

Detailed Description of Preferred Embodiments

Quantum Computer Architecture

Typical quantum computer architectures assume the capability of locally addressing every qubit. Such a requirement is highly challenging to engineer and the achievement of this level of individual quantum control is a major goal in almost every current implementation. The use of such local control methods forces an interaction of the quantum information with very many "classical" control gates, each possibly providing a decohering effect on the quantum information. It is also important that the effects of such control gates on the computer's Hamiltonian remain as "classical" as possible in that they effect a change in the parameters appearing in the system Hamiltonian and do not themselves become entangled with the quantum computer. This criteria of classical gating becomes non-trivial as the length scales of the quantum computer architecture reduces to nanometers.

An alternative architecture is to utilize a small number of identifiable spins, placed in a regular spatial pattern, and to manipulate the quantum information encoded in this spin chain via global addressing techniques. This first of such globally addressed architectures was invented by Lloyd in 1993 [26], and utilized three types of addressable spin arranged in the linear pattern $ABCABCABC$, and where each spin site encodes one logical qubit. In fact this cellular automata design was one of the very earliest quantum computer architectures proposed in the literature. Lloyd showed that such a quantum computer architecture was universal.

Benjamin [27], found a similar architecture which used only two types of identifiable spin species arranged in the alternating linear pattern $ABABAB$. This reduction in spin resources came with an increase in logical encoding: a logical qubit is now encoded into four spin sites with a buffer space of at least four empty spin sites between each logical qubit.

The operation of Benjamin's architecture centers on the ability to implement the global unitary operator, $\hat{A}_f^U$. Denoting the spin up(down) state as $1(0)$, $\hat{A}_f^U$ is the conditional application of the unitary U to the A spins in the alternating spin chain $ABABAB$, depending on the state of A's neighboring B spins. In particular, letting f be the sum of the states of the neighboring B spins, we have $f \in [0,1,2]$ Thus, for example, $\hat{A}_1^U$ is the conditioned application of U to all A spins in the alternating chain which have neighboring B spins that are different from each other, i.e. $f = 1$. One has a similar definition for $\hat{B}_f^U$, for the application of U on all B spins conditioned on their neighboring A spins. The case when $U \sim$ NOT, in $\hat{A}_f^U$ (or $\hat{B}_f^U$), occurs quite frequently in Benjamin's architecture and is shortened to $\hat{A}_f$ (or $\hat{B}_f$).

Benjamin shows in [27], that through a judicious sequence of applications of $\hat{A}_f^U$ and $\hat{B}_f^U$, one can implement single qubit operations and two-qubit CNOT operations and thus the architecture is universal. In particular, to move qubits through the spin chain one applies an alternating pulse sequence of $\hat{A}_1$ followed by $\hat{B}_1$, while the generation of a control-U between two neighboring logical qubits requires ~ 30 global pulses [28]. One can translate all the standard circuit-based quantum algorithms to run with this quantum cellular automata architecture [28]. This programming architecture, though somewhat expensive in terms of

spatial and temporal resources, is ideal for use in systems where the individual control of qubits is difficult and it provides a test-bed for various.

Since Lloyd's and Benjamin's pioneering work little has appeared in the literature with regard to quantum cellular automata designs for quantum computers [29]. There is described below a quantum cellular automata architecture consisting of an alternating linear array of Group V endohedrals, $\mathcal{AB}\mathcal{AB}\mathcal{AB}$ (schematically depicted in Figure 2), for which the full spin Hamiltonian for the pair $\mathcal{AB}$, ($\mathcal{A}$ =^{15}N@C60, $\mathcal{B}$ =^{31}P@C60), can be given as

$$\hat{H}/\hbar = g_e\mu_e B_z \hat{S}_z^{\mathcal{A}} - g_N^{\mathcal{A}}\mu_N B_z \hat{I}_z^{\mathcal{A}} + A^{\mathcal{A}}\hat{S}_z^{\mathcal{A}}\hat{I}_z^{\mathcal{A}}$$

$$+ g_e\mu_e B_z \hat{S}_z^{\mathcal{B}} - g_N^{\mathcal{B}}\mu_N B_z \hat{I}_z^{\mathcal{B}} + A^{\mathcal{B}}\hat{S}_z^{\mathcal{B}}\hat{I}_z^{\mathcal{B}}$$

$$+ J_D \hat{S}_z^{\mathcal{A}}\hat{S}_z^{\mathcal{B}} \qquad (1)$$

where $I(S)$, labels nuclear(electronic) spin, and we have made the secular approximation dropping terms which do not commute with the electronic Zeeman Hamiltonian since $\omega^S_{Larmour} \equiv g_e\mu_e B_z \gg (J_D,\ \omega^I_{Larmour} \equiv g_N\mu_N B_z,\ A)$.

The architecture of such a system will be more thoroughly explored below, but essentially it depends on developing a "quantum algorithm" for generating Benjamin's global operation $\hat{\mathcal{A}}_f^U$ (similarly for $\hat{\mathcal{B}}_f^U$). We first investigate the possibility of implementing $\hat{\mathcal{A}}_f^U$, using the S (electron), spins alone.

The global operation

In this section we consider an alternating spin 1/2 chain of electronic spins $S^{\mathcal{A}}S^{\mathcal{B}}S^{\mathcal{A}}S^{\mathcal{B}}$. We begin by considering the $S^{\mathcal{A}}S^{\mathcal{B}}$ unit alone where $\mathcal{A}$ spin has only one neighboring $\mathcal{B}$ spin. We assume that we know how to perform the controlled operation of applying U to $S^{\mathcal{A}}$, with $S^{\mathcal{B}}$ controlling, an operation we denote by $C(\mathcal{B},\mathcal{A};U)$. We shall describe below the details regarding the sequence of pulses required to execute $C(\mathcal{B},\mathcal{A};U)$. We next consider the case when $\mathcal{A}$ has two neighbors, e.g. $S^{\mathcal{B}}S^{\mathcal{A}}S^{\mathcal{B}}$. Remembering that one cannot separately address an

individual neighboring $\mathcal{B}$ spin one can show that instead of performing $C(\mathcal{B},\mathcal{A};U)$, the above mentioned sequence of pulses now performs

$$\Xi(\mathcal{B},\mathcal{A};U) \equiv C(\mathcal{B}_{\text{on the left}},\mathcal{A};U)C(\mathcal{B}_{\text{on the right}},\mathcal{A};U) \ , \qquad (2)$$

where Eq. (2) defines the function Ξ. One can observe that the case when the desired global operation is $\hat{\mathcal{A}}_1 \equiv \hat{\mathcal{A}}_1^{NOT}$, we have $\hat{\mathcal{A}}_1 = \Xi(\mathcal{B},\mathcal{A};\text{NOT})$.

We now indicate the procedure for implementing $\hat{\mathcal{A}}_2^U$, when the desired $U \sim \exp(i\theta S_x^{\mathcal{A}})$. For ease of notation we define the standard NMR/ESR symbol for $\pi/2$ pulses [30,31,32],

$$[+S_y^{\mathcal{B}}] \equiv \exp(i\frac{\pi}{2}S_y^{\mathcal{B}}) \ , \qquad (3)$$

and the more general rotation through the angle γ about the $z-$axis, for example, by the symbol

$$\{Z_\gamma^{\mathcal{A}}\} \equiv \exp(i\gamma S_z^{\mathcal{A}}) \ . \qquad (4)$$

We find that we can execute $\hat{\mathcal{A}}_2^U$, when $U \sim \exp(i\theta S_x^{\mathcal{A}})$ through the following pulse sequence (read right to left),

$$\begin{aligned}\hat{\mathcal{A}}_2^U = \Xi(\mathcal{B},A;\{X_\delta^{\mathcal{A}}\})\cdot\{X_{\pi/2-\delta}^{\mathcal{A}}\}\cdot\{Z_{-\pi/2}^{\mathcal{A}}\}\cdot\Xi(\mathcal{B},\mathcal{A};\{X_\pi^{\mathcal{A}}\}) \\ \cdot\{Z_{-\pi/2}^{\mathcal{A}}\}\cdot\{X_{\pi/2-\delta}^{\mathcal{A}}\}\cdot\Xi(B,A;\{X_\delta^{\mathcal{A}}\}) \ . \qquad (5)\end{aligned}$$

where $2\delta = \theta$. To implement $\hat{\mathcal{A}}_1^U$ one sets $\delta = \theta$ and replaces the left most term in (5), $\Xi(\mathcal{B},\mathcal{A};\{X_\delta^{\mathcal{A}}\})$, by $\{Z_\pi^{\mathcal{A}}\}$, while to implement $\hat{\mathcal{A}}_0^U$, one applies $\{X_\pi^{\mathcal{B}}\}$ to all the $\mathcal{B}$ spins, then $\hat{\mathcal{A}}_2^U$, and finally flip the $\mathcal{B}$ spins back with $\{X_{-\pi}^{\mathcal{B}}\}$. The above pulse sequence (5), can be easily modified to suit other forms of U besides $\exp(i\theta S_x^{\mathcal{A}})$, however we will find below that the most useful case is when $\theta = \pi$ and $U = \exp(i\pi S_x^{\mathcal{A}}) \sim NOT$ on the $\mathcal{A}$ spin.

All Electronic Quantum Cellular Automata Quantum Computer

From Figure **1**, we can separately address the electronic spins $S^{\mathcal{A}}$ and $S^{\mathcal{B}}$ with a multifrequency selective soft pulse of length $> 20ns$. If we first consider both $S^{\mathcal{A}}$ and $S^{\mathcal{B}}$ to both be spin-$1/2$, then one can use standard pulse encodings of the CNOT [31,32],

$$C(\mathcal{A},\mathcal{B},NOT) = [-S_y^{\mathcal{B}}][\mp S_z^{\mathcal{A}} \mp S_z^{\mathcal{B}}][\pm 2S_z^{\mathcal{A}}S_z^{\mathcal{B}}][+S_y^{\mathcal{B}}]e^{\pm i\pi/4} \quad , \qquad (6)$$

$$C(\mathcal{B},\mathcal{A};NOT) = [-S_y^{\mathcal{A}}][\mp S_z^{\mathcal{A}} \mp S_z^{\mathcal{B}}][\pm 2S_z^{\mathcal{A}}S_z^{\mathcal{B}}][+S_y^{\mathcal{A}}]e^{\pm i\pi/4} \quad , \qquad (7)$$

to generate the operation $\hat{\mathcal{A}}_1$ and $\hat{\mathcal{B}}_1$ of the previous section.

To perform universal quantum computation one must be at least capable of implementing a two-qubit CNOT and a minimal set of one-qubit operations such as the phase gate, the $\pi/8$ gate, and the Hadamard gate. In the quantum cellular automata architecture of Benjamin this means that one must at least be able to implement the global operation $\hat{\mathcal{A}}_f^U$, where U is taken from this minimal set of one qubit gates and the case where $U \sim NOT$. NMR and ESR pulses effectively generate terms in the Hamiltonian which are linear in the spin operators, $I_{x,y,z}$, and $S_{x,y,z}$. In particular, the spin operators when commuted close to form the Pauli algebra. In the case of spin-1/2, the Pauli algebra generates the group SU(2), or all possible spin-1/2 unitaries. Thus one can generate any desired spin-1/2 unitary through a sequence of pulses when acting on an isolated spin. Furthermore, in the case of the alternating chain $\mathcal{AB}\mathcal{AB}\mathcal{AB}$, one can find suitable alterations of (7), when used in (2), and (5), to generate any given unitary U in $\hat{\mathcal{A}}_f^U$ and similarly for $\hat{\mathcal{B}}_f^U$. Thus an all-electronic quantum cellular automata quantum computer architecture (QCAQCA), using a spin-1/2 $\mathcal{AB}\mathcal{AB}\mathcal{AB}$ chain is possible.

Pulsed ESR machines of the type required to generate the required pulse sequences discussed above are of course well known in the art. The spin ½ chains can be implemented as defect centres in crystals (e.g. diamond) or as single electrons trapped in electrostatic traps in ultra-high vacuum. Further embodiments will suggest themselves to the skilled person and new implementations will undoubtedly become available as research in this field progresses.

Endohedral Fullerene-based Quantum Computing

In an alternative embodiment, the invention provides a quantum cellular automata quantum computing architecture (QCAQCA), which can successfully be applied to operate with Group V C60 endohedrals. The QCAQCA design only requires an homogeneous constant magnetic field. More importantly, in the QCAQCA, full scale universal quantum computation with

quantum error correction only requires frequency addressing at a fixed, small number of frequencies, independent of the size of the device. These two advantages mean that a quantum cellular automata based device may be far easier to develop in hardware than any locally addressed architecture.

For the design developed below we exhibit the specific pulse primitives necessary for quantum cellular automata quantum computation. We are also able to estimate rough figures of merit, or number of quantum gates that can be executed in a decoherence time. The estimated figure of merit obtained below compares well with other proposed quantum computer designs. Again, pulsed NMR/ESR machines of the type required to apply the necessary pulse sequences to the array of endohedrally doped fullerenes are well known. An example of such a machine is the Bruker Elexsys ESR machine.

Below we review the properties of $\mathcal{X}$@C60 ($\mathcal{X} = {}^{15}N,\ {}^{31}P$), pertinent for quantum information processing. We briefly outline the essential ingredients of QCAQCA. We develop a number of tools (pulse sequences), for manipulating the Hamiltonian of an alternating linear chain, $\mathcal{AB}\mathcal{AB}\mathcal{AB}$, of these endohedrals where $\mathcal{A}$ =^{15}N@C60 and $\mathcal{B}$ =^{31}P@C60. We consider an architecture which also includes the nuclear spins and show, by developing new gate pulse sequences, that universal quantum computation can be achieved via a quantum cellular automata design. We finally, propose a number of readout techniques that are applicable to the proposed ensemble (a Type-II quantum computer design [9]), and single-issue (or a Type-I quantum computer design [9]), quantum computer design.

Group V Endohedrals

The endohedrals ^{15}N@C60, ^{31}P@C60 and N@C70 all exhibit very sharp ESR spectra [10,11]. This indicates the presence of free electrons within these molecules. It has been further shown, both theoretically and experimentally [12,13,14], that the trapped atom (N or P), sits at the geometric center of the fullerene cage and that the electrons are in a $S = 3/2$ quartet ground state.

The trapped atoms are extreme examples of compressed atoms [15,12], where the electronic wavefunction of the trapped atom is repulsed away from the encompassing carbon cage and

suffers a spatial compression. This unique type of "bonding" leads to significantly higher nuclear-electron wavefunction overlap and thus larger Hyperfine coupling constants than what is found in "free" atoms. For the case of C60 Group V endohedrals, the large symmetry renders this hyperfine coupling highly isotropic. Another consequence of this compression is the virtual lack of any electronic interaction between the trapped atom and the carbon cage. The trapped atom is motionally confined by a harmonic-like potential to the center of the cage. In almost all respects, the trapped atom behaves as a "free" (unbonded) atom, though spatially restricted to be within the fullerene cage. All of the above findings imply that such endohedrals behave as *nanoscopic molecular neutral atom traps*.

The distributed π bonding electrons on the C60 also act as an almost perfect Faraday cage, strongly isolating the electrons of the trapped atom from external electric fields [16]. This latter observation implies that it would require the application intense local electric field gradients $\sim 1V/nm$, in order to alter the Hyperfine coupling constant of the trapped atom. Such an electrostatic addressing scheme has been proposed to address nuclear spin qubits in the Phosphorus donors of the Kane design [3], but with far lower field gradients. Such a scheme would prove very difficult to execute here due to the requirement of such intense electric field gradients.

One very significant advantage of containing the spin site inside a relatively large C60 molecule (diameter $\sim 1nm$), is that such endohedrals can be nano-positioned using current scanning tunneling microscope techniques, and moreover neighboring C60 molecules can be nano-positioned on the Silicon(100)-2x surface to be as close as $\sim 1.1nm$. The C60 molecules, on the Silicon(100)-2x surface, are fixed translationally at room temperature and also rotationally at lower temperatures. Due to the electronic-wavefunction spatial compression experienced by these molecules, the chemistry of the doped Group V fullerene material is practically identical to undoped fullerene. It is therefore possible to self-assemble large organised spin structures using existing well-studied synthetic supra-chemistry techniques [7]. An alternative implementation is to use endohedrally doped fullerenes positioned in nanotubes.

The very sharp ESR spectra from these molecules indicates very long relaxation times and more recent measurements have shown the electronic relaxation times are $T_1 \sim 1s$ at

$T \sim 7°K$, while $T_2 \sim 20\mu s$, $\forall T$ [18]. No nuclear relaxation times have yet been recorded but they are expected to be several orders of magnitude longer than the electronic relaxation times. The measured T_2 time contains contributions from several sources, e.g. unresolved dipolar couplings. The theoretical maximum of T_2, in the complete absence of the unwanted interactions with other paramagnetic impurities, is the relaxation time T_1. Indeed, for the case of Phosphorus defects in isotopically ultra-pure ^{28}Si, the phase relaxation time of the loosely bound Phosphorus electrons can be as long as $T_2 > .1$ msec with $T_1 > 1$ hour [19]. There T_2 is limited by Hyperfine interactions with residual ^{29}Si nuclei [20]. The indicated increase of T_2 towards T_1 in the situation of vanishing spin density [22], is crucial for all current spin-based quantum computer proposals [21,3,4,5,6,7,23]. Achieving such limits will be very challenging. Making these assumptions for the endohedral electrons we expect $T_2 \sim T_1 \sim$ 1sec, at $T \sim 7°K$, with perhaps longer times at lower temperatures.

Such electronic T_1 relaxation times ($\sim$ 1sec), in such complicated molecules is highly unusual and may be unique in all non-crystal hosted spin-sites. Long relaxation times also add to the usefulness of such material as hosts for storing and manipulating quantum information.

An essential ingredient for any quantum information processing is an inter-qubit interaction which can generate entanglement. For Group V C60 endohedrals this cannot be a direct electronic exchange type interaction as the electronic wavefunctions are tightly compressed to be within the C60 cage. The C60's Faraday cage does not restrict magnetic interactions and neighboring endohedrals experience a significant magnetic dipole coupling, $H_D \sim \tilde{J}(1 - 3\cos^2\theta)[3\hat{I}_z\hat{S}_z - \hat{\mathbf{I}} \cdot \hat{\mathbf{S}}] \sim J_D\, \hat{I}_z\hat{S}_z$, in the weak coupling limit. The strength of this dipolar coupling has been estimated to be $J_D \sim$ 50MHz$(1/r^3)$, where r is the separation between the neighboring trapped atoms in the endohedrals measured in nanometers [24], and θ is the angle between $\vec{r}$ and the external $\vec{B}$ field. The Hyperfine coupling constants for ^{15}N@C60, ^{31}P@C60 have been measured [25], and are given in Table 1.

$B_z = 2T$		$A = {}^{15}$N@C60	$B = {}^{31}$P@C60
Electronic Zeeman Energy	$g_e\mu_e B_z$	56GHz	56GHz
Nuclear Zeeman Energy	$g_N\mu_N B_z$	-6.1MHz	34.5MHz
Hyperfine Coupling	A	21.2MHz	138.4MHz

Constant			

Table 1: Table of Hyperfine coupling constants and interaction energies for interacting ^{15}N@C60, ^{31}P@C60 molecules at $B_z = 2T$.

From the above, to a first approximation, the full spin Hamiltonian for the pair $\mathcal{AB}$, ($\mathcal{A}$ =^{15}N@C60, $\mathcal{B}$ =^{31}P@C60), can be given by equation (1) which is repeated here:

$$\hat{H}/h = g_e\mu_e B_z \hat{S}_z^{\mathcal{A}} - g_N^{\mathcal{A}}\mu_N B_z \hat{I}_z^{\mathcal{A}} + A^{\mathcal{A}}\hat{S}_z^{\mathcal{A}}\hat{I}_z^{\mathcal{A}}$$

$$+ g_e\mu_e B_z \hat{S}_z^{\mathcal{B}} - g_N^{\mathcal{B}}\mu_N B_z \hat{I}_z^{\mathcal{B}} + A^{\mathcal{B}}\hat{S}_z^{\mathcal{B}}\hat{I}_z^{\mathcal{B}}$$

$$+ J_D \hat{S}_z^{\mathcal{A}}\hat{S}_z^{\mathcal{B}} \qquad (1)$$

where $I(S)$, labels nuclear(electronic) spin, and we have made the secular approximation dropping terms which do not commute with the electronic Zeeman Hamiltonian since $\omega^S_{Larmour} \equiv g_e\mu_e B_z \gg (J_D,\ \omega^I_{Larmour} \equiv g_N\mu_N B_z,\ A)$. The individual ESR and NMR spectra of these molecules are simulated in Figure **1**, and have been measured in [11].

Quantum Cellular Automata

The endohedrals ^{15}N@C60 and ^{31}P@C60, unlike the all-electronic spin ½ chains for which the global unitary operators were developed above, possess electron spin $S = 3/2$ and the application of Benjamin's QCAQCA is not as straightforward.

One possibility is to consider the four electronic levels of the electron spin with $S = 3/2$ to constitute a qu-dit with $d = 4$. Multi-level quantum computation has been proposed elsewhere [33], but this invention does not extend Benjamin's formulation of the spin-1/2 QCAQCA to operate with qu-dits. Indeed, as shown below there are reasons to believe that that such an extension may not be possible within the confines of NMR and ESR.

Remaining with qubits we instead propose to encode a qubit into the four levels of a spin 3/2 in two ways: an "inner qubit" $\{|m_s = \pm 1/2\rangle\}$, and an "outer qubit" $\{|m_s = \pm 3/2\rangle\}$. By a small alteration of (7), one can obtain

$$C_{inner}(S^{\mathcal{A}}, S^{\mathcal{B}}; NOT) = C_{outer}(\overline{S_{\mathcal{A}}}, S^{\mathcal{B}}; NOT) = [S_y^{\mathcal{B}}][-S_z^{\mathcal{A}} - S_z^{\mathcal{B}}][+2S_z^{\mathcal{A}}S_z^{\mathcal{B}}][-S_y^{\mathcal{B}}]e^{+i\pi/4} \quad , \tag{8}$$

$$C_{inner}(S^{\mathcal{B}}, S^{\mathcal{A}}; NOT) = C_{outer}(\overline{S_{\mathcal{B}}}, S^{\mathcal{A}}; NOT) = [S_y^{\mathcal{A}}][-S_z^{\mathcal{A}} - S_z^{\mathcal{B}}][+2S_z^{\mathcal{A}}S_z^{\mathcal{B}}][-S_y^{\mathcal{A}}]e^{\pm i\pi/4} \quad , \tag{9}$$

where C_{inner} is a $CNOT$ on the Hilbert space spanned by the inner qubits, and similarly for C_{outer}, $\overline{S^A} = NOT(S^A)$, and we have used the spin-3/2 representations of the $SU(2)$ group. Armed with this one can easily construct the Benjamin global operations $\hat{A}_1$ and $\hat{B}_1$ on the inner qubit subspace. One can further construct (as discussed below), the global operations $\hat{A}_f^{NOT}$, (and similarly $\hat{B}_f^{NOT}$), for $f = 0$, 1 and $f = 2$, the operations most frequently used in the quantum cellular automata quantum computation.

However one finds that one cannot generate all the one-qubit gates required for universal quantum computation. As above, ESR pulses essentially generate terms in the Hamiltonian that are linear in the spin operators and again these terms commute to form a Pauli algebra. Evolution under such terms lead to dynamics that resides in the group generated by this Pauli algebra (or $SU(2)$). However, since now we have $S = 3/2$, this $SU(2)$ is merely a subgroup of the full group of unitaries that can act on a spin-3/2, but as long as the system Hamiltonian is linear in the spin operators we need only to consider the dynamics within the $SU(2)$ subgroup. Normally a unitary operation $U \in SU(2) \subset SU(4)$ will not factor into unitary operations on the inner and outer qubit subspaces. However if U is diagonal in the $|m_s\rangle$ basis it can so factor and with this one can find pulse sequences to implement $\hat{A}_f^U$ where U is a phase gate, and the $\pi/8$ gate but crucially not the Hadamard gate. Thus an all electronic-QCAQCA with a system Hamiltonian which is linear in the spin operators and where $S > 1/2$ seems not possible.

One way of implementing $SU(2)$ operations on the qubit subspaces and one which is well known in NMR and ESR is to introduce terms in the system Hamiltonian which are not linear in the spin operators. Such terms lie in the full spin-3/2 algebra and the generated unitaries no

longer lie in the $SU(2)$ subgroup but in the much larger $SU(4)$ group. One effect of such nonlinear terms, for example Zero-Field-Splitting terms: $H_{ZFS} \propto S_z^2$, can be to lift the degeneracy of the microwave transition frequencies between the $|m_s\rangle \leftrightarrow |m_s+1\rangle$. This allows one to frequency address the transition $|m_s=-1/2\rangle \leftrightarrow |m_s=+1/2\rangle$, or the inner qubit subspace, and directly implement $SU(2)$ operations on this subspace. This allows the generation of arbitrary one-qubit unitaries U [34]. However, this solution frustrates the coherence transfer portion, $[+2S_z^{\mathcal{A}}S_z^{\mathcal{B}}]$, of the pulse sequence (8), and (9), and thus the construction of the global QCAQCA operator $\hat{A}_f^U$. This can be seen by realising that to obtain a $[+2S_z^{\mathcal{A}}S_z^{\mathcal{B}}]$ pulse one must effectively cancel out all the terms in the system Hamiltonian bar the term $S_z^{\mathcal{A}}S_z^{\mathcal{B}}$. As standard in NMR and ESR one does this cancellation through "average Hamiltonian" theory [35], via the application of various $SU(2)$ unitaries by RF or MW pulses. As long as the system evolution remains within the $SU(2)$ subspace such an averaging out can be achieved. However when terms nonlinear in the spin operators are introduced into the system Hamiltonian no application of $SU(2)$ unitaries can, in general, average out the resulting "nonlinear" evolution (i.e. in the average Hamiltonian theory nonlinear terms in the Hamiltonian will almost always average to other nonlinear terms), and thus the generation of $[+2S_z^{\mathcal{A}}S_z^{\mathcal{B}}]$, and from this $\hat{A}_f^U$, is not possible.

Thus we have found that when operating on an $\mathcal{ABABAB}$, spin-3/2 chain with ESR pulses one cannot generate all of the necessary global operations required for universal quantum computation. The present invention, however, demonstrates that the combination of nuclear and electronic spins within the chain can provide the necessary framework for the global operations.

Nuclear-electron quantum cellular automata

^{15}N@C60 and ^{31}P@C60 both have nuclear spin-1/2. In this section we assume that the quantum information is stored in the nuclear spins of the dopant atoms in the $\mathcal{ABABA}$ chain. This has the significant advantage that the nuclear spin relaxation times are typically longer than the electronic spins by several orders of magnitude. As the nuclei only are coupled via the Hyperfine interaction to the electrons, one can, via a suitable RF and MW pulse sequence, cancel out this Hyperfine interaction with high precision. This allows the nuclei to act as a

quantum memory and store the quantum information for very long periods of time in between processing.

To execute the Benjamin global operation $\hat{A}_f^U$ we essentially use the inner electronic qubits as a local "bus" for the quantum information stored in the nuclei. The procedure can be thought of as a quantum algorithm for the generation of the global operation and consists of several steps which are pictorially represented in Figure **3**.

The algorithm starts with the inner electronic qubit bus in the ground state ($|m_s\rangle = |-1/2\rangle$ for all molecules), and this bus is returned to the ground state after implementing the global operation $\hat{A}_f^U$. We first (a) assume that we have an arbitrary pattern of quantum information written onto the nuclear spins of the $\mathcal{A}$ and $\mathcal{B}$ molecules with the electrons set as above. We then, (b) swap the quantum information of all the $\mathcal{B}$ molecules from their nuclei to their inner electronic qubits. We then (c) tag those $\mathcal{A}$ molecules which will receive the unitary operation U in $\hat{A}_f^U$ by flipping the state of the electronic qubit of all the $\mathcal{A}$ molecules conditioned on the state of it's neighboring $\mathcal{B}$ electronic qubits. We then (d) undo (b) by swapping the quantum information back into the $\mathcal{B}$ nuclei from their electrons.

At this point all the inner electronic qubits are back in their ground states except for the "tagged" $\mathcal{A}$ molecules. We then, (e) perform a controlled- U operation on the nuclear qubits of *all the molecules* using their inner electronic qubits as the control. Finally (f), we undo the operations (d), (c) and (b). The system is then ready for the execution of the next global operation.

One restriction we make in the following is that we rule out the use of selective pulses on the nuclear spins of the Nitrogen and Phosphorus. From Figure **1**, to execute such selective pulses would require RF pulses of very long duration to frequency differentiate between the NMR transitions of the Nitrogen and Phosphorus. Such slow nuclear pulse sequences would lead to very long gates times. We will therefore not allow ourselves to use such selective nuclear pulse sequences and instead make use of fast "hard" nuclear pulse sequences [36]. We do allow selective addressing of the electronic transitions of the Nitrogen and Phosphorus as these pulse

sequences are much shorter in duration. With this restriction however we are still able to design all the pulse sequences that are required to carry out the steps (b)-(e), above. The resulting combined total pulse sequence is somewhat lengthy but could be substantially shortened by applying the principles of optimal control theory [37].

We now expand on the above steps (a)-(e), in detail. In section (A) below we describe the initialization of the spin-chain. In section (B) we design the *SWAP* pulse sequence required for step (b). In section (C) we design the electronic pulse sequence to implement the conditional operation required in step (c), and finally in section (D) we outline the execution of the controlled- U needed in step (d). In section (E) we discuss the undoing of the previous steps (b)-(d), while in section (F) we provide some estimates of the pulse durations and logical QCA gate times.

A:- Initialization

The QCA architecture may be implemented on an ensemble (Type-II) or single-issue (Type-I), quantum computer. The achievement of high nuclear polarizations has proved to be a major obstacle in NMR quantum computation. It remains a source of difficulty here as well. Polarizing the electrons is far easier, and one can achieve a difference in the ground to excited electronic populations of $\epsilon \sim 0.999$, at a temperature of $1^{\circ}K$ and $B \sim 10$T. Even when multiple spins are tensored to produce a pseudo-pure state, with such high individual polarizations one can still achieve a pseudo-pure state with a purity on the order of $\epsilon \sim .998$, with 1000 spins at these temperatures and magnetic fields. This polarization can be transferred to the nuclei via an INEPT pulse sequence [38]. To repump the electronic polarization and achieve a subset of completely spin (nuclear and electron), polarized molecules one could consider two chains of equal length: an $\mathcal{AB}\mathcal{AB}\cdots$ chain and a $\mathcal{CDCD}\cdots$ chain where all $\mathcal{A}$, $\mathcal{B}$, $\mathcal{C}$, and $\mathcal{D}$ are globally addressable. Since at 1°K and $B = 10$T, half of the spins (the electrons), are completely polarised, one can consider an $\mathcal{AB}\mathcal{AB}\cdots\mathcal{AB}\mathcal{AB}\mathcal{X}\mathcal{CDCD}\cdots\mathcal{CDCD}$ super-chain where $\mathcal{X}$ has a different resonant frequency yet again. One can then use a spin cooling quantum algorithm [39], to efficiently spin cool *all* the nuclear and electronic spins on one side of $\mathcal{X}$ (i.e. $\mathcal{X}$ acts as a spin gate). One would then switch off the interaction between the two sub-chains at $\mathcal{X}$ and use the spin polarised half chain to perform the quantum computation. Such a design would be suitable for a Type-II (ensemble), quantum computer. Alternatively, in the case of a Type-I quantum computer one can replace the $\mathcal{CDCD}$ chain with an $\mathcal{AB}\mathcal{AB}$ chain and place the

readouts on the polarised half chain. More practically any Type-I quantum computer will require a single-spin readout of the electronic spins of the endohedral atoms. Such a readout may also serve to initialize the electronic qubits. We discuss possibilities for a single-spin readout further below.

B:- Nuclear-Electronic *SWAP*

A crucial ingredient in the above mentioned quantum algorithm to generate $\hat{A}_f^U$ is the Hyperfine *SWAP*. This operation performs a logical swap between a qubit stored in the nuclear spin and a qubit stored in the electron spin. Below we find two types of Hyperfine *SWAP*, one that performs the swap using the inner electronic qubit and one that uses the outer electronic qubit. For the most part we will use the former type of swap but we will find later that the latter swap, which incorporates the outer electronic qubit, may be of significant use in the problem of qubit readout and we discuss this below.

To develop the pulse sequence for the Hyperfine *SWAP* it is useful to break down the *SWAP* operation into three *CNOT* operations. Denoting $SWAP(I:S)$, we have, $SWAP(I:S) = CNOT(I;S)CNOT(S;I)CNOT(I;S)$, where $CNOT(I;S)$ is the controlled *NOT* for I controlling S. In our case $I = 1/2$ while $S = 3/2$. Substituting the spin-3/2 representations for S into the standard spin-$1/2$ *CNOT* pulse sequence (7), fails to yield a proper *CNOT* operation. One instead must make reference to the two cases of a *CNOT* with respect to the inner and outer qubits of S. With this one can find:

$$CNOT_{outer}(I;S) = [S_y][\mp S_z \mp I_z][\pm 2S_zI_z][-S_y]e^{\pm i\pi/4} \ ,$$

$$CNOT_{outer}(S;I) = [I_y][\pm S_z \pm I_z][\pm 2S_zI_z][-I_y]e^{\pm i\pi/4} \ , \qquad (10)$$

while

$$CNOT_{inner}(I;S) = [S_y][\mp S_z \mp I_z][\pm 2S_zI_z][-S_y]e^{\pm i\pi/4} \ ,$$

$$CNOT_{inner}(S;I) = [-I_y][\mp S_z \mp I_z][\pm 2S_z I_z][I_y]e^{\pm i\pi/4} \quad . \qquad (11)$$

With these one can derive

$$SWAP_{inner}(I:S) = [I_y][+2I_zS_z][S_y - I_y][S_x - I_x][+2I_zS_z][I_x - S_x][+2I_zS_z][I_y]e^{-i\pi/4}; \quad , \qquad (12)$$

$$SWAP_{outer}(I:S) = [-I_y][+2I_zS_z][-I_y - S_y][-I_x - S_x][+2I_zS_z][S_x + I_x][+2I_zS_z][-I_y]e^{+3i\pi/4} \quad , \qquad (13)$$

and the related pulse sequences are graphically shown in Figure **4**. We note for later the curious case of (13), where we have in some sense "amplified" the magnetic signature of the qubit from a $\Delta m_I = \pm 1$, transition to a $\Delta m_S = \pm 3$, transition. In the following we will restrict ourselves to the inner electronic qubit subspace and thus (12).

Having found a $SWAP$ operation between the nuclear and inner electronic qubits of either molecule we now must show how one can adapt the sequence (12), to swap out only the $\mathcal{B}$ qubits while leaving the $\mathcal{A}$ nuclear qubits alone. We now consider the case of two coupled $\mathcal{AB}$ molecules with the Hamiltonian (1). The desired selective swap action can be achieved by replacing the $[+2I_zS_z]$ terms in (12), with the pulse sequence shown in Figure **5**. This new pulse sequence effectively averages out the Hyperfine coupling interaction in the $\mathcal{A}$ molecules thus turning off the action of the Hyperfine $CNOT$ and $SWAP$ gates for these molecules. The Hyperfine interaction for the $\mathcal{B}$ molecules is left intact by the pulse sequence but is reduced in magnitude thus lengthening their Hyperfine gate durations.

The black pulses in Fig. 5 are π pulses and the duration of the entire sequence is matched to yield $[+2I_z^{\mathcal{B}}S_z^{\mathcal{B}}]$ in (13). The gray pulses are fast hard X_π pulses which are required to extend the duration of the $[2I_zS_z]$ for the case when swapping between the nuclear and electronic spin in ^{31}P@C60. By placing these pulses at the points $(m-1)/(4m)$, and $(3m+1)/(4m)$, in each third section as shown, we can extend the pulse sequence by a factor m. Setting $m = 6$ brings the

^{31}P@C60 *SWAP* to be $\sim$ 20MHz, and thus long enough for the electronic spin selective pulses to operate on $S^{\mathcal{A}}$ and $S^{\mathcal{B}}$.

This particular pulse sequence has a number of advantages, the most important of which is that we do not selectively address the nuclear spins and thus can apply fast hard pulses to $I^{\mathcal{A}}$ and $I^{\mathcal{B}}$ simultaneously. We only take advantage of the selective addressing of the electronic spins of $\mathcal{A}$ and $\mathcal{B}$ as outlined previously. Alternatively, one can use soft multi-frequency nuclear pulses in the following to approximate the hard nuclear pulse. In more detail, from [40,41], the action of this pulse sequence is to remove to all orders (within the secular approximation made previously), all interactions between $S^{\mathcal{A}} \leftrightarrow S^{\mathcal{B}}$ and $S^{\mathcal{A}} \leftrightarrow I^{\mathcal{A}}$. This sequence also removes all the Zeeman terms in the $\mathcal{AB}$ Hamiltonian and one is thus left with $\hat{H}/h \sim A^{\mathcal{B}} \hat{S}_z^{\mathcal{B}} \hat{I}_z^{\mathcal{B}}$. When inserted into (12), the effect is to swap the qubit that was stored in $I^{\mathcal{B}}$, into the inner electronic qubit of $S^{\mathcal{B}}$. As mentioned above, the quantum information stored in $I^{\mathcal{A}}$ is not swapped into $S^{\mathcal{A}}$, but these spins do receive the local unitary transformation, $[S_y^{\mathcal{A}}][I_y^{\mathcal{A}}]$. The local unitary $[S_y^{\mathcal{A}}]$ is removed with a spin selective electronic pulse $[-S_y^{\mathcal{A}}]$, however we cannot remove the $[I_y^{\mathcal{A}}]$ without performing a spin selective nuclear pulse, an operation we wish to avoid. We will see however, that this extraneous local operation on $I^{\mathcal{A}}$ is not important for the tagging of the $\mathcal{A}$ molecules and furthermore the operation will be "undone" in step (d) (c.f. Figure **3**).

C:- Electronic tagging of f

Summarizing the previous steps: we have now swapped out the nuclear qubits of the $\mathcal{B}$ molecules in the $\mathcal{ABABABAB}$ chain into their inner electronic qubits. Additionally, all the inner electronic qubits of the $\mathcal{A}$ molecules are in their ground states $|m_s\rangle = |-1/2\rangle$, i.e. we are at step (b) in Figure **3**. We will now electronically "tag" those $\mathcal{A}$ molecules targeted by the global operation $\hat{A}_f^U$.

More precisely, we wish to flip the state of the $\mathcal{A}$ inner electronic qubit subject to the function f, with the control being $\mathcal{A}$'s nearest neighbor $\mathcal{B}$'s inner electronic qubits. We noted at the end of the section entitled "quantum cellular automata", that many inter-molecular electronic unitaries cannot be achieved with $SU(2)$ pulses. However, the case of $f = 1$ is simply the operation $\Xi(\mathcal{B}, \mathcal{A}; NOT)$, where one uses (8), for the $CNOT$ in the inner electronic qubit

subspace. The case $f = 2$ is more difficult and one must make full use of the construction given in (5), to obtain the following pulse sequence

$$\Xi(\mathcal{B},\mathcal{A};\sqrt{NOT})\cdot\{Z^{\mathcal{A}}_{-\pi/2}\}\cdot\Xi(\mathcal{B},\mathcal{A};\sqrt{NOT})$$
$$\cdot\{Z^{\mathcal{A}}_{-\pi/2}\}\cdot\Xi(\mathcal{B},\mathcal{A};\sqrt{NOT})\,e^{3i\pi/4}\quad . \qquad (14)$$

where $\Xi(\mathcal{B},\mathcal{A};\sqrt{NOT}) \equiv C(S^{\mathcal{B}},S^{\mathcal{A}};\Sigma)^2$, (see (2)), and

$$C(S^{\mathcal{B}},S^{\mathcal{A}};\Sigma) \equiv e^{i\frac{1}{2}\pi S^{\mathcal{A}}_Y} e^{-i\frac{1}{4}\pi(S^{\mathcal{A}}_Z+S^{\mathcal{B}}_Z-2S^{\mathcal{A}}_Z S^{\mathcal{B}}_Z)} e^{-i\frac{1}{2}\pi S^{\mathcal{A}}_Y} e^{i\pi/4}\quad . \qquad (15)$$

With this pulse sequence one achieves the required spin flip of the $\mathcal{A}$ molecule's inner electronic qubit up to a phase. This global phase is unimportant as it will be removed in step (e), when we undo the unitaries. Finally the case $f = 0$ is dealt with by first flipping all $\mathcal{B}$ inner electronic qubits, then using the $f = 2$ operation above, and then flipping back. In the case of Figure **3**, we have chosen to implement the tag $f = 1$ operation in step (c). Once we have set the electronic tag on the appropriate $\mathcal{A}$ molecules we "undo" the $SWAP$, returning $\mathcal{B}$'s quantum information back into its nuclei and $\mathcal{B}$'s inner electronic qubits to the ground state, arriving at step (d) in Figure **3**.

D:- Implementing U

We now can implement **any** desired unitary on the flagged $\mathcal{A}$ qubits. The construction of this operation is well known [42], and consists of applying hard pulses [36], to *all* of the $\mathcal{A}$ and $\mathcal{B}$ and nuclei interspersed by CNOT gates between the inner electronic qubits and nuclear qubits of all the molecules. More precisely, the controlled execution of any given unitary operation on the nuclear spin I controlled by the inner electronic qubit S on all the molecules may be written as

$$C(S,I;U) = D\,C(I,S;X)\,E\,C(I,S;X)\,F\quad , \qquad (16)$$

$$U \equiv e^{i\alpha}R_z(\beta)R_y(\gamma)R_z(\delta)$$

$$= e^{i\alpha} DXEXF \quad . \qquad (17)$$

In (16), β, γ, and δ are the Euler angles of the desired nuclear $SU(2)$ operation, $C(I,S;X)$ is the Hyperfine control-NOT given in (11), the nuclear rotation operators are given by $R_\delta(\theta) \equiv \exp(-i\theta\,\delta/2)$, where $\delta = x, y, z$ and standard pulse sequences for these spin rotations can be found in [38]. Further $D \equiv R_z(\beta)R_y(\gamma/2)$, $E = R_y(-\gamma/2)R_z(-(\delta+\beta)/2)$, $F = R_z((\delta-\beta)/2)$, $X \sim NOT$, and α is a phase. Crucially one can show that $DEF = I$. From this one can see that the action of the sequence (16), on the nuclear spin is unity when the inner electronic qubit is not set. When the inner electronic qubit is set however, the action of (16), is to execute U from (17), on the nuclear spin up to the phase α. One then finally applies the local unitary $\exp(i\alpha(S_z^{\mathcal{A}} + S_z^{\mathcal{B}}))$, to all molecules to yield the final phase factor α in (17). With this one has the very powerful capability of applying *any* desired single-qubit unitary to the nuclear qubits of the tagged $\mathcal{A}$ molecules. However, the typical operation in the QCAQCA is $\hat{\mathcal{A}}_f$, and this can be executed more simply by a Hyperfine $CNOT$ between the electronic and nuclear qubits of all the molecules. In Figure **3**, we illustrate the application of $\hat{\mathcal{A}}_1$ in subfigure (e).

E:- Undoing the unitaries

Following the arguments made above, we execute step (e), that is: once we have implemented the desired unitary on the $\mathcal{A}$ nuclear qubits we "undo" steps (b), (c) and (d). We $SWAP$ the nuclear qubit into the electrons on all $\mathcal{B}$ molecules, undo the tagging of the $\mathcal{A}$ molecules, and then $SWAP$ the quantum information back into the nuclei of the $\mathcal{B}$ molecules. The system is left with all the inner electronic qubits in their ground states while the nuclear qubits have received the global operation $\hat{\mathcal{A}}_f^U$.

F:- Gate duration

As we noted above, the resulting pulse sequence is quite lengthy. However it may be possible to compress many of the above operations. Also all nuclear pulses are fast hard pulses of little duration [43], while the primary slowdown arises from the nuclear-electronic $SWAP$ whose duration is limited by the value of the Hyperfine coupling constant of ^{15}N@C60 ($\sim$ 20MHz), and the separation of the spectral lines of the $\mathcal{A}$ and $\mathcal{B}$ molecules in the ESR spectrum of Fig. **1** ($\sim$ 50MHz). The typical QCAQCA global operation, $\hat{\mathcal{A}}_f$, entails a pulse sequence in which the

terms $[+a_z b_z]$, occurs 15 times, each with an average duration of $50ns$, thus roughly bringing the cycle time of the global operation down to $1\mu s$. As noted above, the simplest quantum logic gate in the QCAQCA scheme requires ~ 30 global operations. This finally brings the cycle time for logical gates in the resulting QCAQCA to be roughly $\sim 30\mu s$.

As noted above, one has $T_1 \sim 1s$ at $T = 7^{\circ}K$, and $T_2 \sim 20\mu s$ for concentrated samples of ^{15}N@C60 Group-V endohedral material. As mentioned above, recent experiments have indicated a dependence on concentration for T_2 and it is commonly expected in all current spin-based quantum computer implementations that T_2 will rise towards the value of T_1 in the limit of zero spin concentration. If $T_2 \sim 1s$ then one can expect on average $10,000 - 30,000$, logical operations within this dephasing time (figure of merit). Indeed, at temperatures lower than 7°K one might be able to achieve far greater figures of merit as the decoherence and dephasing times increase. A figure of merit of 10^4 compares very favorably with most alternative proposed implementations for quantum information processors.

Readout

One of the most challenging aspects of any solid-state implementation is that of readout. We first discuss the possibilities for an ensemble readout for the QCAQCA and later a single-spin readout for a Type-I implementation.

In the original scheme of Lloyd [26], the only spin sites which could be individually addressed were those at either end of the chain as these spins were frequency differentiated by having a single neighbor. This is also the situation here. However, if these two sites were the only readout sites on the chain then the architecture would not be scalable in the presence of noise. One ensemble readout possibility is to attach an electrically isolated paramagnetic adduct to every B molecule, (Gd@C82 may be a possibility). Such readout sites would typically possess short relaxation times and one would have to isolate such sites from the operation of the primary processor using ESR pulses. It should be possible within the cellular automata architecture to selectively readout the state of a single qubit, that is, to transfer the state of a given logical qubit into the readout site. This can be done by adapting the single-qubit unitary operator U, pulse scheme in [27]. This pulse sequence is arranged so that a logical qubit (which is usually encoded in four spins, $ABAB$), gets driven into the state of a single spin

which is then subject to a unitary operation, U, through the application of the global operation (say $\hat{B}_f^U$, when the qubit has been forced into the spin state of a $\mathcal{B}$ molecule). The spin neighborhood of this target $\mathcal{B}$ spin is arranged so that this global operation only effects the state of that spin alone with an appropriate choice for f. For readout one could instead apply an operation $\hat{B}_f^{SWAP}$, which swaps out the state of the spin into the readout site. This would be read and then $SWAP$ed back.

For a Type-I quantum information processor based on the $\mathcal{ABAB}$ chain of ^{15}N@C60 and ^{31}P@C60 one must be capable of performing a single electron spin readout. We suggest a number of possible technologies that may be capable of performing such a readout below. Before mentioning these we return to Equation (13). There we noticed that this pulse sequence was able to $SWAP$ the qubit between the highest and lowest weight subspaces of the nuclear and electronic spins, $I = 1/2$ and $S = 3/2$, and in the process increase the detectable magnetic signature by a factor ~ 1000.

We will now further enquire whether there exists similar pulse sequences which could further $SWAP$ out the quantum information now stored in the outer electronic qubit into a separate coupled electronic system of larger spin. This could be very advantageous, for example, for the purposes of coupling into the spin-chain, a nano-molecular magnet with a spin of $\sim 10 - 30$ as a potential readout site [44]. As the $SWAP$ gate is built from $CNOT$ gates we can focus on the latter. Further, the pulse sequences must only consist of higher spin representations of the Pauli group. There may be many such pulse sequences and we here present one set of sequences. The ones given below perform a $CNOT$ between the highest and lowest weight subspaces of spins I and S. We set $I = a/2$ and $S = b/2$, where $b \geq a$ and both a and b are odd integers. Letting $\alpha = [a/2]$ and $\beta = [b/2]$, where $[]$ is the integer part of the fraction, we can find $CNOT$ pulses for the following four cases:

$$\alpha \text{ even}, \ \beta \text{ even}: \ C_(I,S;NOT) = [-S_y][-S_z - I_z][+2S_zI_z][S_y]e^{+i\pi/4} \ , \tag{18}$$

$$C_(S,I;NOT) = [-I_y][-S_z - I_z][+2S_zI_z][I_y]e^{+i\pi/4} \ , \tag{19}$$

$$\alpha \text{ odd, } \beta \text{ odd}: \; C_(I,S;NOT) = [-S_y][+S_z + I_z][+2S_zI_z][S_y]e^{+i\pi/4} \;, \tag{20}$$

$$C_(S,I;NOT) = [-I_y][+S_z + I_z][+2S_zI_z][+I_y]e^{+i\pi/4} \;, \tag{21}$$

$$\alpha \text{ odd, } \beta \text{ even}: \; C_(I,S;NOT) = [S_y][+S_z + I_z][+2S_zI_z][-S_y]e^{+i\pi/4} \;, \tag{22}$$

$$C_(S,I;NOT) = [I_y][-S_z - I_z][+2S_zI_z][-I_y]e^{+i\pi/4} \;, \tag{23}$$

$$\alpha \text{ even, } \beta \text{ odd}: \; C_(I,S;NOT) = [S_y][-S_z - I_z][+2S_zI_z][-S_y]e^{+i\pi/4} \;, \tag{24}$$

$$C_(S,I;NOT) = [I_y][+S_z + I_z][+2S_zI_z][-I_y]e^{+i\pi/4} \;. \tag{25}$$

A Type-I quantum computer design will require the capability of single qubit readout and this translates in our case to the capability of reading out the spin state of the endohedral electrons. One can classify the various readout methods into the general categories (i) force, (ii) electric, and (iii) optical, measurement techniques. As was mentioned before, since the electronic wavefunction of the trapped atom is totally confined within the C60 cage, spin measurement techniques that involve the physical transport of this spin outside the molecule are not possible here. Some techniques, such as ODMR (optically detected magnetic resonance), have so far not proved possible with ^{15}N@C60 and ^{31}P@C60, and thus the addition of separate readout sites which can be dynamically coupled and decoupled from the primary processor via NMR/ESR pulses are warranted.

Possible techniques in the above mentioned categories include (i) Magnetic Resonance Force Microscopy (MRFM) [47]; (iia) Micro-Squids, a technology which is already capable of discriminating a $\Delta m_S = 30$ [46]; (iib) Scanning-Tunneling-Microscope ESR, a technique which, though not well understood, has yielded single molecule ESR spectroscopy of iron impurities in Silicon [45], and in single BDPA molecules on Silicon [48]. (iic) A single molecule endohedral fullerene single electron transistor [49]. This is a very challenging technology which has yielded a single electron tunneling current through a C60 molecule with an electro-mechanical coupling to the quantized motion of the entire molecule. Performing such an experiment with ^{15}N@C60 may yield endohedral spin information; (iiia) Magnetic coupling of the endohedral electronic spin to a solid-state paramagnetic optical dipole such as a nanocrystaline N-V center in diamond. The optical paramagnetic center can then be probed via

optical shelving techniques [50]; (iiib) ODMR via a magnetic coupling to a paramagnetic endohedral adduct which is chemically bonded to the $^{15}N@C60$ molecule. For use with ODMR the adduct endohedral should ideally possesses an optical transition in the visible spectrum such as $Er_xSc_{3-x}N@C80$ [51] .

The techniques suggested above are, in some cases, already at the single electron detection level (though not capable of detecting the spin orientation), while the out-coupling of the quantum information into a large-spin system may allow the techniques of micro-Squids and MRFM as they presently stand to act as a readout of a single endohedral electronic spin.

The direction taken in the present invention with regard to the construction of a quantum information processor is to follow as closely as possible the system Hamiltonian that nature provides. The globally addressed approach has very significant advantages over the local gating approach. Global addressing avoids the buildup of numerous decoherence pathways associated with the effects of the local gates on the processor. Global addressing also avoids the very significant problem of the scaling up of the external resources required to execute local gating, e.g. numerous metallic contacts or multi-frequency MW/RF generators with increasing bandwidths. Although it may be true that for local gating, the external resources required increase polynomially with the number of qubits in the processor, such an overhead may not be experimentally feasible as the size of the processor grows large.

In some sense the technical complexities involved in the construction and operation of local gating are transferred into the quantum cellular automata "software". As shown above, the detailed operation of a quantum cellular automata quantum computer architecture does not follow the standard quantum circuit model. This should not be seen as a disadvantage as all quantum circuit algorithms can be "compiled" to run on a QCAQCA with a polynomial overhead [27]. Indeed the QCAQCA may be able to run programs that do not follow the quantum circuit model (see [52] for an example of a non-circuit quantum program in another architecture). Furthermore, as the fundamental quantum operations are implemented via the very well developed methods of NMR and ESR, the fidelity of software execution is heightened. The QCAQCA also has the very important property that it can execute quantum

computations in parallel, a characteristic necessary for the ultimate scalability of the architecture.

We have considered the endohedral fullerene material ^{15}N@C60 and ^{31}P@C60 and argued that the system Hamiltonians and interactions present are sufficient to implement universal quantum computation via a quantum cellular automata architecture. Following the DiVincenzo criteria: (i) we argued that the Group-V endohedral materials behave as essentially electrostatically isolated nanoscopic molecular neutral atom traps that can be physically manipulated with relative ease using STM techniques and perhaps may be self-assembled using fullerene supra-chemistry. (ii) the electronic decoherence times are perhaps the longest seen in any molecular system, of the order of seconds at temperatures of ~ 7°K, which is also an upper limit for the electronic dephasing time. The nuclear decoherence times have not yet been measured but they are expected to be several orders of magnitude longer than the electronic decoherence times. (iii) The complete polarization of both the nuclear and electronic computational spins is feasible as half of the spins (electrons), within the entire system are completely polarised at moderate conditions of temperature and magnetic field strength. There are efficient cooling schemes exist to shuffle the unpolarized spins away from the computational spins. (iv) entanglement can be generated via the inter-molecule magnetic dipole interaction, the strength of which has been measured to be $\sim$ 50MHz. Armed with the two species ^{15}N@C60 and ^{31}P@C60, we showed that one has sufficient control to implement a two-component quantum cellular automata quantum computing architecture storing the quantum information in the nuclear spins while using the electrons as a local bus. We further found that the expected "figure of merit" compares very well with other proposed solid-state quantum computer designs. We also discovered pulse sequences that *SWAP*ed the quantum information between the highest and lowest weight spaces of two spins of different size, e.g. $S = 1/2 \leftrightarrow S = 11/2$. These sequences could prove useful for out-coupling the quantum information into a spin readout system with large spin.

DiVincenzo's final criterion: (v) an efficient single qubit readout, is perhaps the most difficult challenge for any solid-state based quantum computer design. We have proposed various possible ensemble and single-issue (Type-I), readout technologies many of which are themselves the subjects of intense study. The ideas presented here combine the tremendous power of NMR and ESR science together with the very "clean", and almost atomic, systems

presented by the endohedrals $^{15}N@C60$ and $^{31}P@C60$. These, married with supra-molecular chemistry, provide a very real physical implementation of a quantum information processor.

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Claims:

1. A method of quantum computing in a system comprising a plurality of spin systems of two distinct types A and B arrayed in an ABABAB... sequence, wherein each A-type spin system comprises a first spin subsystem A1 and a second spin subsystem A2 coupled to one another, and each B-type spin system comprises a first spin subsystem B1 and a second spin subsystem B2 coupled to one another, wherein the first spin subsystems (A1,B1) of neighbouring A and B-type spin systems are substantially isolated from one another and the second spin subsystems (A2,B2) of neighbouring A and B-type spin systems are coupled to one another, said method comprising the steps of:

c) encoding quantum information on the first spin subsystems (A1,B1); and

d) employing the second spin subsystems (A2,B2) as a local bus for the information encoded on the first spin subsystems.

2. A method of quantum computing as claimed in claim 1, wherein the step of employing the second spin subsystems (A2,B2) as a local bus comprises the steps of:

a) transferring the information encoded in the B1 spin subsystems to the B2 spin subsystems via a first spin swapping operation;

b) tagging a subset of the A2 spin subsystems, with said tagging being effected by manipulating those A2 spin subsystems for which B2 spin subsystems of the neighbouring B-type spin systems fulfil a predetermined condition;

c) transferring the information encoded in the B2 spin subsystems to the B1 spin subsystems via a second spin swapping operation; and

d) performing a spin manipulation on a subset of first spin subsystems (A1,B1), with said manipulation being targeted to those first spin subsystems (A1,B1) for which the associated second spin subsystem (A2,B2) fulfils a predetermined condition.

3. A method as claimed in claim 2, wherein the predetermined condition of the associated second spin subsystem in step (d) according to which the first spin subsystems are targeted is the condition of being tagged or untagged following step (b).

4. A method as claimed in claim 2 or 3, further comprising an initialisation step of

polarising a group of second spin subsystems to a substantially common state prior to performing said first spin swapping operation.

5. A method as claimed in any of claims 2 to 4, further comprising the step of returning said second spin subsystems (A2,B2) to their initial configurations after performing spin manipulation in step (d).

6. A method as claimed in claim 4, wherein the step of returning said second spin subsystems (A2,B2) to their initial configurations comprises:

a) transferring the information encoded in the B1 spin subsystems to the B2 spin subsystems via a third spin swapping operation;
b) reversing the tagging of said subset of A2 spin subsystems; and
c) transferring the information encoded in the B2 spin subsystems back to the B1 spin subsystems via a fourth spin swapping operation.

7. A method of quantum computing as claimed in any preceding claim, wherein said first spin subsystems (A1,B1) are spin ½ subsystems.

8. A method of quantum computing as claimed in any preceding claim, wherein said first spin subsystems (A1,B1) are a nuclear spin subsystems I_A,I_B.

9. A method as claimed in any preceding claim wherein said second spin subsystems (A2,B2) are spin n/2 subsystems where n is an odd integer.

10. A method of quantum computing as claimed in any preceding claim, wherein said second spin subsystems (A2,B2) are electron spin subsystems S_A,S_B.

11. A method of quantum computing as claimed in claim 10 when dependent on claim 8, wherein the coupling between the nuclear and electron spin subsystems of a spin system is via the hyperfine interaction.

12. A method of quantum computing as claimed in any preceding claim, when dependent on claim 2, wherein said spin swapping operations are hyperfine spin swapping

operations.

13. A method of quantum computing as claimed in claim 10 or any claim dependent thereon, wherein said electron spin subsystems S_A and S_B of neighbouring A and B-type spin systems are coupled to one another via a magnetic dipole interaction.

14. A method as claimed in claim 2 or any claim dependent thereon, wherein said first spin subsystems (A1,B1) are nuclear spin subsystems I_A,I_B having spin I=1/2, and said second spin subsystems (A2,B2) are electron spin subsystems S_A,S_B of free electrons each having S=3/2, wherein a qubit in the electronic spin subsystems is encoded as an electronic inner qubit defined as {|ms=±1/2}, and said nuclear spin subsystems and electron spin subsystems within a spin system (I_A,S_A; I_B,S_B) are coupled via the hyperfine interaction.

15. A method as claimed in claim 14, wherein the step of employing the electron spins as a local bus for the information encoded on the nuclear spins comprises performing one or more hyperfine spin swapping operations between the nuclear spins I and electron spins S by applying NMR/ESR pulses according to the swap operation equation:

$$SWAP_{inner}(I:S) = [I_y][+2I_zS_z][S_y - I_y][S_x - I_x][+2I_zS_z][I_x - S_x][+2I_zS_z][I_y]e^{-i\pi/4}$$

16. A method as claimed in claim 15, wherein a sequence of NMR/ESR pulses as represented in Fig. 4 is applied to the spin systems to effect said hyperfine swap operation.

17. A method as claimed in claim 2 or any claim dependent thereon, wherein said first spin subsystems (A1,B1) are nuclear spin subsystems I_A,I_B having spin I=1/2, and said second spin subsystems (A2,B2) are electron spin subsystems S_A,S_B of free electrons each having S=3/2, wherein a qubit in the electronic spin subsystems is encoded as an electronic outer qubit defined as {|ms=±3/2}, and said nuclear spin subsystems and electron spin subsystems within a spin system (I_A,S_A; I_B,S_B) are coupled via the hyperfine interaction.

18. A method as claimed in claim 17, wherein the step of employing the electron spins as a local bus for the information encoded on the nuclear spins comprises performing one or

more hyperfine spin swapping operations between the nuclear spins I and electron spins S according to the swap operation equation:

$$SWAP_{outer}(I:S) = [-I_y][+2I_zS_z][-I_y - S_y][-I_x - S_x][+2I_zS_z][S_x + I_x][+2I_zS_z][-I_y]e^{+3i\pi/4}$$

19. A method as claimed in claim 15 or 18, wherein said swap operation is selectively applied to one of said spin system types only (A or B only) by applying additional NMR/ESR pulses to decouple the hyperfine interaction of the other of said distinct qubit types.

20. A method as claimed in claim 18, wherein wherein a sequnece of NMR/ESR pulses as represented in Fig. 5 is applied to the spin systems to decouple the hyperfine interaction of the other of said distinct spin system types.

21. A method as claimed in any preceding claim, wherein each spin system is implemented as a fullerene molecule having an endohedral atom or molecule.

22. A method as claimed in claim 21, wherein said distinct types of spin system are obtained by providing fullerenes with two different endohedral atoms or molecules therein.

23. A method as claimed in claim 22, wherein said different endohedral atoms or molecules are different atoms each having a free electron and each located in the same periodic group.

24. A method as claimed in claim 23, wherein one of said spin system types is implemented as ^{15}N@C60 and the other of said spin system types is implemented as ^{31}P@C60.

25. A method as claimed in any one of claims 21 to 24, wherein said fullerenes are positioned in said ABABAB... array on a substrate.

26. A method as claimed in claim 25, wherein said substrate is silicon.

27. A method of quantum computing in a system comprising a plurality of spin systems of two distinct types A and B arrayed in an $ABABAB$ sequence, wherein each spin system

comprises a spin ½ entity, said method comprising performing one or more global unitary operations $\hat{A}_f^U$ on the $\mathcal{A}$ spin systems, wherein:

$\hat{A}_f^U$ is the conditional application of the unitary U when $U \sim NOT$ to the $\mathcal{A}$ spins depending on the state of $\mathcal{A}$'s neighboring $\mathcal{B}$ spins;

f is the sum of the states of the neighboring $\mathcal{B}$ spins, with spin up(down) defined as 1(0) such that $f \in [0,1,2]$;

and wherein:

said global unitary operations are performed by applying pulse sequences according to one of the following sequence notations (a)-(c):

a) $\hat{A}_2^U = \Xi(\mathcal{B}, A; \{X_\delta^{\mathcal{A}}\}) \cdot \{X_{\pi/2-\delta}^{\mathcal{A}}\} \cdot \{Z_{-\pi/2}^{\mathcal{A}}\} \cdot \Xi(\mathcal{B}, \mathcal{A}; \{X_\pi^{\mathcal{A}}\})\{Z_{-\pi/2}^{\mathcal{A}}\} \cdot \{X_{\pi/2-\delta}^{\mathcal{A}}\} \cdot \Xi(B, A; \{X_\delta^{\mathcal{A}}\})$. read from right to left where $2\delta = \theta$; or

b) $\hat{A}_1^U = \{Z_\pi{}^{\mathrm{A}}\} \cdot \{X_{\pi/2-\delta}^{\mathcal{A}}\} \cdot \{Z_{-\pi/2}^{\mathcal{A}}\} \cdot \Xi(\mathcal{B}, \mathcal{A}; \{X_\pi^{\mathcal{A}}\})\{Z_{-\pi/2}^{\mathcal{A}}\} \cdot \{X_{\pi/2-\delta}^{\mathcal{A}}\} \cdot \Xi(B, A; \{X_\delta^{\mathcal{A}}\})$. read from right to left where $\delta = \theta$; or

c) $\hat{A}_0^U$ implemented as an application of $\{X_\pi^{\mathcal{B}}\}$ to all the $\mathcal{B}$ spins, followed by $\hat{A}_2^U$, followed by an application of $\{X_\pi^{\mathcal{B}}\}$ to all the $\mathcal{B}$ spins;

wherein the controlled operation of applying U to an $\mathcal{A}$ spin with left and right $\mathcal{B}$ neighbours such that the $\mathcal{B}$ spins control the unitary application is denoted by $C(\mathcal{B}, \mathcal{A}; U)$. and the function Ξ is in turn defined by the equation:

$$\Xi(\mathcal{B}, \mathcal{A}; U) \equiv C(\mathcal{B}_{\text{on the left}}, \mathcal{A}; U) C(\mathcal{B}_{\text{on the right}}, \mathcal{A}; U) \ ,$$

and wherein in equations (a)-(c) the NMR/ESR notation for $\pi/2$ pulses used is:

$$[+S_y^{\mathcal{B}}] \equiv \exp(i\frac{\pi}{2} S_y^{\mathcal{B}}) \ ,$$

and rotation through the angle γ about the z–axis, for example, is denoted as:

$$\{Z_\gamma^{\mathcal{A}}\} \equiv \exp(i\gamma S_z^{\mathcal{A}}) \ .$$

28. A method as claimed in claim 27, wherein $U = \exp(i\theta S_x^{\mathcal{A}})$.

29. A method as claimed in claim 28, wherein $\theta = \pi$.

30. A method as claimed in any one of claims 27-29, further comprising performing one or more global unitary operations $\hat{B}_f^U$ on the $\mathcal{B}$ spin systems, said unitary operations being defined for the $\mathcal{B}$ spins depending on the state of $\mathcal{B}$'s neighboring $\mathcal{A}$ spins in terms identical to the unitary operations $\hat{A}_f^U$ other than the substitution of the symbol $\mathcal{B}$ for $\mathcal{A}$ and vice versa at each occurrence of said symbols in each foregoing equation and definition.

31. A method as claimed in any preceding claim, wherein said spin ½ entities A and B have an Ising-like interaction defined as $J_D \hat{S}_z^A \hat{S}_z^B$, where J_D is a measure of the magnetic dipole coupling strength between the A and B entities.

32. A quantum computer comprising:

a) a plurality of entities providing quantum spin systems of two distinct types A and B arrayed in an ABABAB... sequence, wherein

each A-type spin system comprises a first spin subsystem A1 and a second spin subsystem A2 coupled to one another, and each B-type spin system comprises a first spin subsystem B1 and a second spin subsystem B2 coupled to one another,

the first spin subsystems (A1,B1) of neighbouring A and B-type spin systems are substantially isolated from one another and the second spin subsystems (A2,B2) of neighbouring A and B-type spin systems are coupled to one another,

b) an NMR/ESR pulse generator associated with said array of entities for generating and applying pulses to said array of entities; and

c) means for reading the spin state of one or more of said entities.

33. A quantum computer as claimed in claim 31, wherein each spin system is implemented as a fullerene molecule having an endohedral atom or molecule.

34. A quantum computer as claimed in claim 30 or 31, further comprising a computer program associated with said NMR/ESR generator, said computer program including instruction which when executed are effective to cause said NMR/ESR generator to generate pulses effective to:

a) encode quantum information on the first spin subsystems (A1,B1); and

b) employ the second spin subsystems (A2,B2) as a local bus for the information encoded on the first spin subsystems.

35. A quantum computer comprising:

a) a plurality of entities providing quantum spin systems of two distinct types A and B arrayed in an ABABAB... sequence, wherein each spin system comprises a spin ½ entity copled to its two neighbours

b) an NMR/ESR pulse generator associated with said array of entities for generating and applying said pulses to said array of entities; and

c) means for reading the spin state of one or more of said entities.

36. A quantum computer as claimed in claim 35, further comprising a computer program associated with said NMR/ESR generator, said computer program including instruction which when executed are effective to cause said NMR/ESR generator to gemerate pulses effective to perform one or more global unitary operations $\hat{\mathcal{A}}_f^U$ on the $\mathcal{A}$ spin systems, wherein:

$\hat{\mathcal{A}}_f^U$ is the conditional application of the unitary U when $U \sim NOT$ to the $\mathcal{A}$ spins depending on the state of $\mathcal{A}$'s neighboring $\mathcal{B}$ spins;

f is the sum of the states of the neighboring $\mathcal{B}$ spins, with spin up(down) defined as 1(0) such that $f \in [0,1,2]$;

and wherein:

said global unitary operations are performed by applying pulse sequences according to one of the following sequence notations (a)-(c):

a) $\hat{\mathcal{A}}_2^U = \Xi(\mathcal{B}, \mathcal{A}; \{X_\delta^{\mathcal{A}}\}) \cdot \{X_{\pi/2-\delta}^{\mathcal{A}}\} \cdot \{Z_{-\pi/2}^{\mathcal{A}}\} \cdot \Xi(\mathcal{B}, \mathcal{A}; \{X_\pi^{\mathcal{A}}\})\{Z_{-\pi/2}^{\mathcal{A}}\} \cdot \{X_{\pi/2-\delta}^{\mathcal{A}}\} \cdot \Xi(B, A; \{X_\delta^{\mathcal{A}}\})$. read from right to left where $2\delta = \theta$; or

b) $\hat{\mathcal{A}}_1^U = \{Z_\pi^{\mathcal{A}}\} \cdot \{X_{\pi/2-\delta}^{\mathcal{A}}\} \cdot \{Z_{-\pi/2}^{\mathcal{A}}\} \cdot \Xi(\mathcal{B}, \mathcal{A}; \{X_\pi^{\mathcal{A}}\})\{Z_{-\pi/2}^{\mathcal{A}}\} \cdot \{X_{\pi/2-\delta}^{\mathcal{A}}\} \cdot \Xi(B, A; \{X_\delta^{\mathcal{A}}\})$. read from right to left where $\delta = \theta$; or

c) $\hat{\mathcal{A}}_0^U$ implemented as an application of $\{X_\pi^{\mathcal{B}}\}$ to all the $\mathcal{B}$ spins, followed by $\hat{\mathcal{A}}_2^U$, followed by an application of $\{X_\pi^{\mathcal{B}}\}$ to all the $\mathcal{B}$ spins;

wherein the controlled operation of applying U to an $\mathcal{A}$ spin with left and right $\mathcal{B}$ neighbours such that the $\mathcal{B}$ spins control the unitary application is denoted by $C(\mathcal{B},\mathcal{A};U)$. and the function Ξ is in turn defined by the equation:

$$\Xi(\mathcal{B},\mathcal{A};U) \equiv C(\mathcal{B}_{\text{on the left}},\mathcal{A};U)C(\mathcal{B}_{\text{on the right}},\mathcal{A};U) \ ,$$

and wherein in equations (a)-(c) the NMR/ESR notation for $\pi/2$ pulses used is:

$$[+S_y^{\mathcal{B}}] \equiv \exp(i\frac{\pi}{2}S_y^{\mathcal{B}}) \ ,$$

and rotation through the angle γ about the $z-$axis, for example, is denoted as:

$$\{Z_\gamma^{\mathcal{A}}\} \equiv \exp(i\gamma S_z^{\mathcal{A}}) \ .$$

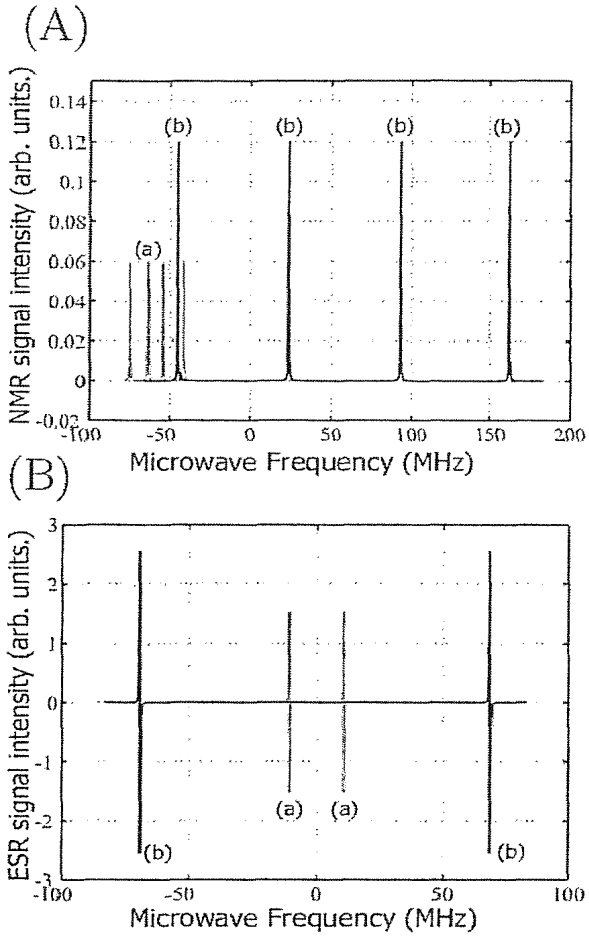

Figure 1

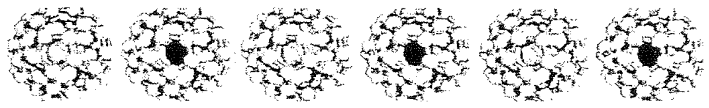

Figure 2

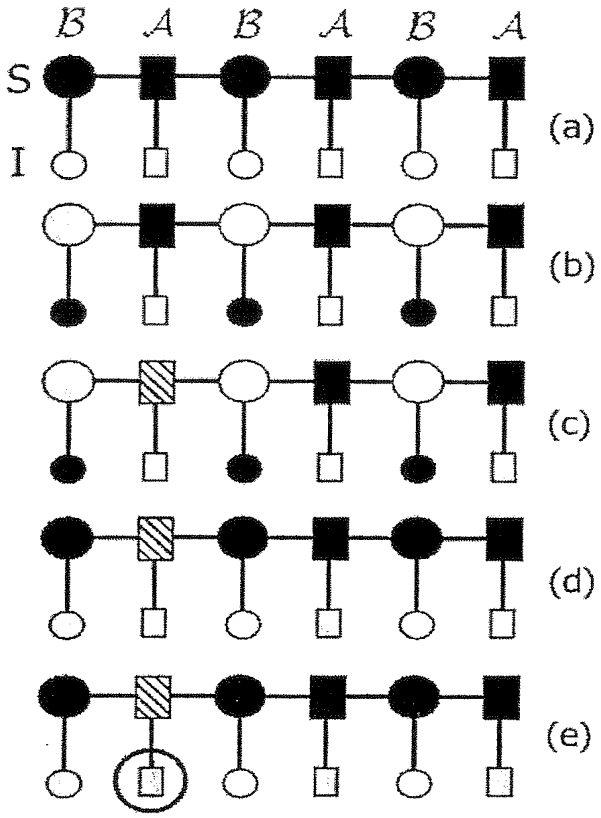

Figure 3

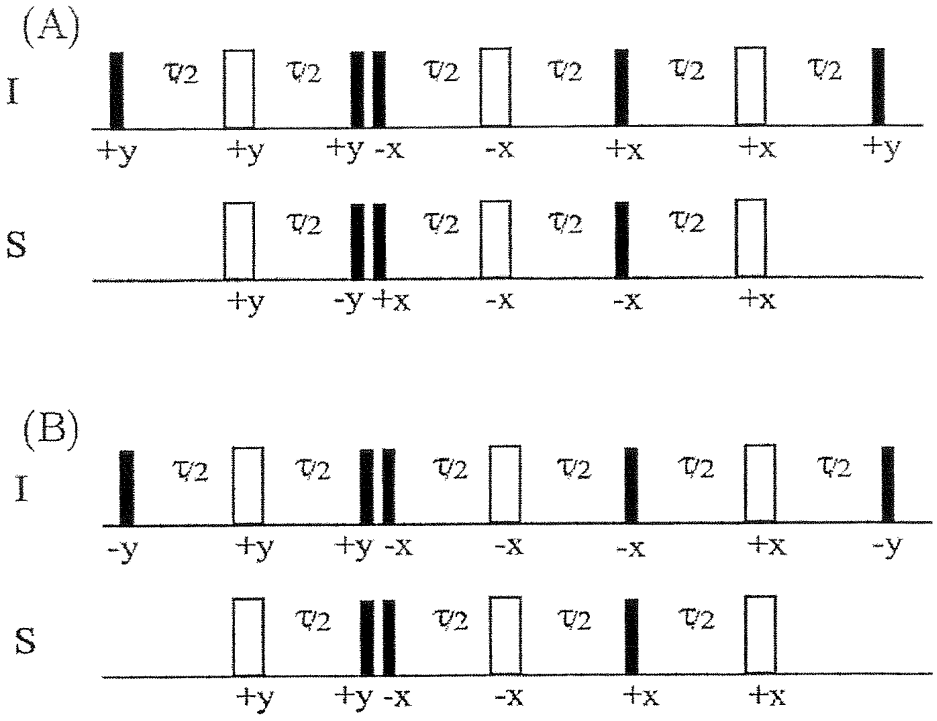

Figure 4

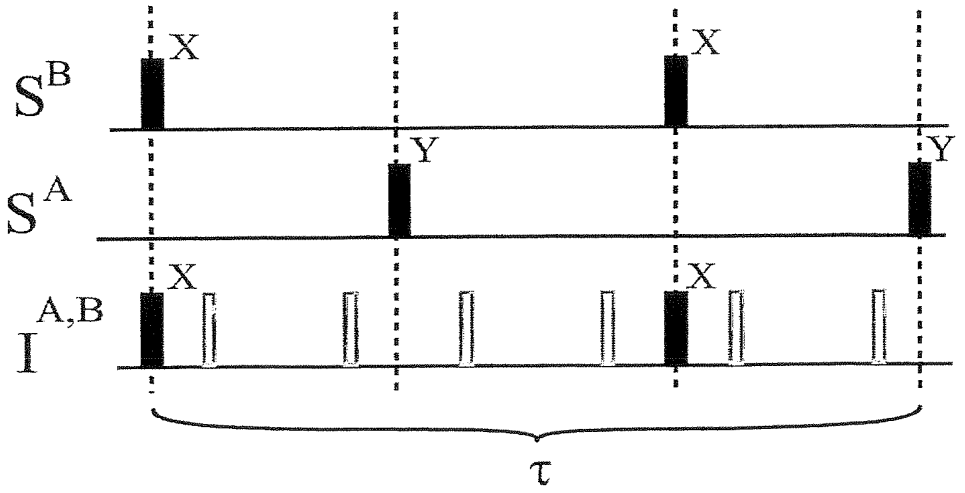

Figure 5

INTERNATIONAL SEARCH REPORT

International Application No
PCT/EP 03/02997

A. CLASSIFICATION OF SUBJECT MATTER
IPC 7 G06N1/00

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 7 G06N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)
INSPEC, EPO-Internal, WPI Data, COMPENDEX, IBM-TDB

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	SEONGJUN PARK ET AL: "Endo-fullerene and doped diamond nanocrystallite-based models of qubits for solid-state quantum computers" JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY, MARCH 2001, AMERICAN SCIENTIFIC PUBLISHERS, USA, vol. 1, no. 1, pages 75-81, XP002243575 ISSN: 1533-4880 abstract the whole document --- -/--	1,7-11, 13,14, 21-26, 32-35

[X] Further documents are listed in the continuation of box C.

[ ] Patent family members are listed in annex.

° Special categories of cited documents :

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier document but published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
6 June 2003	09. 07. 2003

Name and mailing address of the ISA	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	JENNY FORSS /EÖ

Form PCT/ISA/210 (second sheet) (July 1992)

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	BENJAMIN S C: "Simple pulses for universal quantum computation with a Heisenberg ABAB chain" PHYSICAL REVIEW A (ATOMIC, MOLECULAR, AND OPTICAL PHYSICS), NOV. 2001, APS THROUGH AIP, USA, vol. 64, no. 5, pages 054303/1-3, XP002243576 ISSN: 1050-2947 figure 2 abstract ---	1,7-11, 13,14, 21-26, 32-35
A	HARNEIT W: "Fullerene-based electron-spin quantum computer" PHYSICAL REVIEW A (ATOMIC, MOLECULAR, AND OPTICAL PHYSICS), MARCH 2002, APS THROUGH AIP, USA, vol. 65, no. 3, pages 032322/1-6, XP002243577 ISSN: 1050-2947 figures 1,5 abstract ---	1-36
P,X	HARNEIT W ET AL: "Architectures for a spin quantum computer based on endohedral fullerenes" 275. WE-HERAEUS-SEMINAR: HARDWARE CONCEPTS FOR QUANTUM COMPUTING, BAD HONNEF, GERMANY, 13-15 MAY 2002, vol. 233, no. 3, pages 453-461, XP002243578 Physica Status Solidi B, Oct. 2002, Wiley-VCH, Germany ISSN: 0370-1972 the whole document -----	1-36